Name ____ AP Chemistry

Molecular Geometry & Polarity

Molecular Geometry

A key to understanding the wide range of physical and chemical properties of substances is recognizing that atoms combine with other atoms to form molecules or compounds and that the shape or geometry of a collection of atoms strongly affects the properties of that substance. One reason this occurs is because the distribution of charge in a molecule affects many properties of the substance. For example, if the negative change is concentrated in one region of a molecule its' properties will be widely different than if the charge is distributed evenly throughout the entire molecule.

The valence shell electron-pair repulsion (VSEPR) model predicts the geometries of molecules and polyatomic ions. The structure around the central atom is determined by minimizing electron-pair repulsions. Bonding and nonbonding pairs of electrons are positioned as far apart as possible. Nonbonding or lone pairs of electrons require more room than bonding pairs and tend to compress the angle between bonding pairs.

Today you are going to work through the "Molecular Shapes" PhET simulation to learn how to predict the different geometries.

1) Go to https://phet.colorado.edu/en/simulation/molecule-shapes. Click on "Run Now."
2) On the upper right corner, there is an option to add 'bonding' and 'lone pairs.' Below these, there is a box entitled 'Options.' Click on 'Show Bond Angles.'
3) In the bottom left corner, there is a box entitled 'Name.' Click to show both the Molecule Geometry and Electron Geometry.
4) Initially there is a molecule with a central atom with two atoms bonded to it and no lone pairs. Record the Molecule and Electron Geometry in the chart below. Then record the bond angle
5) Add a single bond to the central atom. Record the Molecule and Electron Geometry and the bond angles. Sketch a rough image of what the molecule looks like.
6) Remove the single bond and add a lone pair. Again record the Molecule and Electron Geometry and the bond angles. Sketch a rough image of what the molecule looks like, including the lone pairs.
7) Complete the rest of the chart, recording the Electron and Molecule Geometry and bond angles. Sketch a rough image of what the molecule looks like, including the lone pairs.

Number of Total Electrons around Central Atom	Bond-ing Pairs	Lone Pairs	Electron Geometry	Molecule Geometry	Bond Angles	Sketch of Molecule
2	2	0				
3	3	0				
3	2	1				
4	4	0				
4	3	1				
4	2	2				
5	5	0				
5	4	1				
5	3	2				
5	2	3				
6	6	0				
6	5	1				
6	4	2				

8) Looking at the chart you created, what do you think the difference between electron geometry and molecule geometry is? More specifically, what is each including or not including, such as the number of bonded pairs, number of lone pairs, etc.?

9) Click on ‘Remove all,’ located underneath the ‘Lone Pair’ box. Add one lone pair and a double bond and a triple bond. What is the Electron and Molecule Geometry and bond angles?

10) How does your answer compare to your answer in the third row of your chart above? Does VSEPR distinguish between single, double, or triple bonds?

Molecular Polarity

Based on the difference in electronegativity, the type of bond can be determined along with the polarity of the bond. With a covalent bond, the electrons are shared but the more electronegative molecule will keep the electrons more, creating a difference within the bond. You are going to work with the “Molecule Polarity” today to learn more about how the electronegativity difference can determine the type of bond and how the polarity of a bond is.

1) Go to https://phet.colorado.edu/en/simulation/molecule-polarity. Click on “Run Now.”
2) Click to view all three options in the first box on the right-side of the screen along with choosing ‘Electron Density’ under Surface.
3) Complete the table below by changing the electronegativity for either atom A or atom B.

Atom A	**Atom B**	**Bond Character (covalent/ionic/ between)**	**Sketch of A + B with partial charges and dipole arrow**	**Describe/draw Surface**
Between	Between			

Between	More			
Less	More			

4) There are partial charges, δ^- and δ^+, are displayed on the molecule if there is a difference of electronegativity. What do you think each of these mean?
   δ^-

   δ^+

5) When these partial charges occur, an arrow is also shown. This arrow describes a dipole moment. Define what a dipole moment is in your own words and how you draw the arrow (such as where is the arrowhead located).

6) How does the density around a partial positive compare to the density of a partial negative?

7) A bond is characterized as ionic or covalent by comparing the differences between two atoms' electronegativities. Describe an ionic bond in terms of the atoms' electronegativity values and what has happened to the electrons involved in the bond.

8) Describe a covalent bond in terms of the atoms' electronegativity values and what has happened to the electrons involved in the bond.

9) Additionally covalent bonds can be separated into polar covalent and nonpolar covalent. What would have to be the case for a bond to be nonpolar covalent?

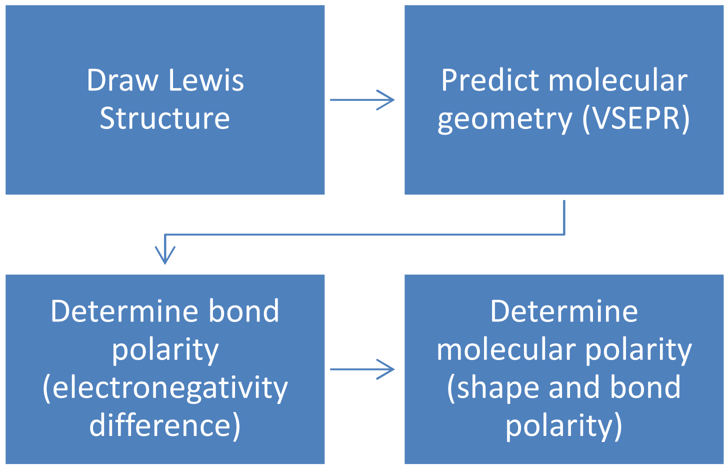
10) Click on “Three Atoms” tab at the top of the simulation window.

In addition to bond polarity (represented by the bond dipole moment), the entire molecule may be polar (represented by the molecular dipole moment). It is this molecular dipole that determines the polarity of the molecule and how it interacts with other molecules and its environment. The molecular dipole is found using vector addition, adding the bond dipoles together; think a tug-of-war.

11) Take some time and adjust each of the atom's locations and electronegativity values several times. Observe how the bond dipoles (between A-B and B-C) add to produce a molecular dipole.
12) How might a molecule with two strong bond dipoles have no molecular dipole at all?

13) How might a molecule have a very strong molecular dipole?

Putting it All Together



Molecule	Lewis Structure	Molecular Geometry	Is there a molecule dipole?
N_2			
H_2O			
BF_3			
HCN			
CH_2F_2			

*Make a prediction first and then check your answer in the "Real Molecules" tab.

**Adapted from "Molarity Geometry and Polarity" by Ted Clark, "Outlining Bonding versus Shape Polarity" by Amanda Zullo, and "Molecular Polarity PhET Lab" by Chris Bires (from phet.colorado.edu).